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Diethyl 2,3-bis(4-methoxybenzoyl)succinate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.056
wR factor = 0.151
Data-to-parameter ratio = 13.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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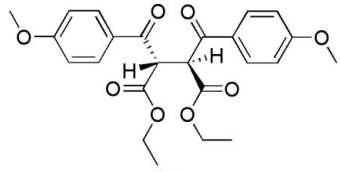
The title molecule, $C_{24}H_{26}O_8$, has approximate twofold rotation symmetry and the crystal structure is stabilized by intermolecular C—H···π interactions.

Comment

1,4-Diketones are versatile intermediates for the synthesis of some natural products containing cyclopentanone and furan rings (McMurry & Meiton, 1971; Ito *et al.*, 1975, 1977). The structures of the 1,4-diketones (2*RS*,3*SR*)-diethyl 2,3-bis(3,4,5-trimethoxybenzoyl)succinate (Meng & Wu, 2005) and (2*RS*,3*SR*)-diethyl 2,3-bis(3,4-dimethoxy-benzoyl)succinate (Wang *et al.*, 2005) have been reported recently and shown to be *meso* isomers. As a continuation of our interest in this area, the structure of the title compound, (I), is presented.



(I)

The X-ray crystallographic analysis shows (I) to possess an approximate twofold axis (Fig. 1 and Table 1) in contrast to the above-mentioned structures. The main feature of the crystal packing are C—H···π interactions, as summarized in Table 2.

Experimental

Compound (I) was synthesized as reported previously (Wu *et al.*, 1997). Crystals appropriate for data collection were obtained by slow evaporation of a methanol–ethyl acetate (1:1 *v*/*v*) solution of (I).

Crystal data

$C_{24}H_{26}O_8$
M_r = 442.45
Monoclinic, $P2_1/c$
a = 13.079 (5) Å
b = 9.611 (4) Å
c = 18.572 (7) Å
β = 102.757 (8)°
V = 2276.9 (15) Å^3
Z = 4
D_x = 1.291 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 3551 reflections
θ = 2.4–23.5°
μ = 0.10 mm^{-1}
T = 292 (2) K
Block, colorless
0.30 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
11106 measured reflections
4009 independent reflections
3133 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°
h = −13 → 15
k = −11 → 9
l = −16 → 22

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.151$
$S = 1.04$
4009 reflections
293 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.8894P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C9—C10	1.532 (3)		
C8—C9—C10	110.75 (19)	C9—C10—C11	111.02 (18)
C8—C9—C19	108.68 (19)	C9—C10—C22	110.53 (18)
C10—C9—C19	109.62 (18)	C11—C10—C22	107.06 (18)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of benzene ring C2–C7.

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···$Cg1^{i}$	0.93	2.92	3.743 (3)	148
C16—H16···$Cg1^{ii}$	0.93	3.00	3.689 (4)	132

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

The methyl H atoms were constrained to an ideal geometry, with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.96 Å for aromatic and 0.97 Å for methylene H atoms, and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

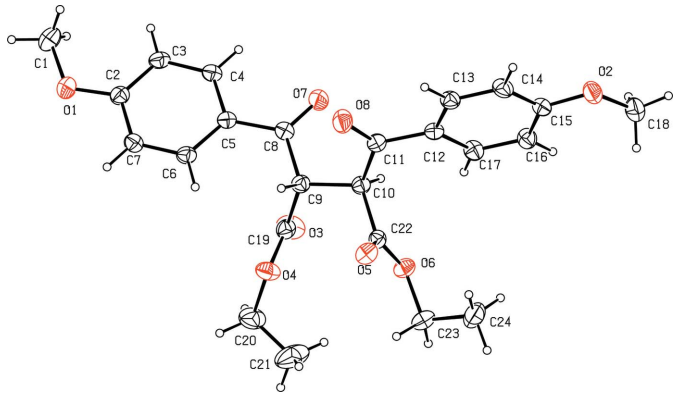


Figure 1
View of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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References

Bruker (2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Ito, Y., Konoike, T., Harada, T. & Saegusa, T. (1977). *J. Am. Chem. Soc.* **99**, 1487–1493.
Ito, Y. Konoike, T. & Saegusa, T. (1975). *J. Am. Chem. Soc.* **97**, 649–651.
McMurry, J. E. & Meiton, J. (1971). *J. Am. Chem. Soc.* **93**, 5309–5311.
Meng, X.-G. & Wu, A.-X. (2005). *Acta Cryst.* E**61**, o3117–o3118.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wang, Z.-G., Chen, A.-H., Hu, S.-L. & Wu, A.-X. (2005). *Acta Cryst.* E**61**, o3172–o3173.
Wu, A., Zhao, Y., Chen, N. & Pan, X. (1997). *Synth. Commun.* **27**, 331–336.